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Elastic Behavior of an Atomic Lattice Under Large Volumetric Strains: The Quasi-Harmonic Idealization

by Steven B. Segletes

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Elastic Behavior of an Atomic Lattice Under Large Volumetric Strains: The Quasi-Harmonic Idealization

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Abstract

The implications of Segletes' recent equation of state are examined, when idealized to the condition defined as quasi-harmonicity. Results indicate that at large volumetric strains, a proportionality no longer holds, in general, between the volumetric and vibrational stiffnesses. The governing relation between these two stiffnesses is presented and is a function of the characteristic frequency of the lattice, alternately expressed in terms of the lattice spacing. It is further shown that the quasi-harmonic idealization of Segletes' equation will approach the harmonic approximation in the limit.

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1. Background

The harmonic approximation has been the traditional method to analyze atomic vibrations and lattice behavior, dating back to Planck. Several years later, in the early 1900s, Einstein, Debye, and Born and von Karman [1] used the approximation to develop theories of lattice specific heat. In the years that followed, Brillouin [2] also employed the harmonic approximation to analyze wave propagation in lattice structures.

In the harmonic approximation, atoms vibrate with sinusoidal motion. In order for an atom within the crystal lattice to retain this harmonic behavior, the specific potential energy well of the lattice, $E_{pot}(r)$, must be parabolic in shape, where r is the coordinate of the atom in question within the lattice. Specifically, $\Delta E_{pot} \sim (r - r_0)^2$. Under these conditions, the restoring force to the atom is proportional to its displacement from the rest position, and the resulting oscillatory motion of the atom is sinusoidal—that is to say, harmonic. The harmonic motion of an atom has a single frequency associated with it, ω_0 , and that frequency is calculable, just as in macroscopic vibration theory, by the relation $\omega_0^2 = (-\partial P/\partial r) / M$, where M is the mass of the atom, P is the restoring force, and $-\partial P/\partial r$ is the local spring constant in the direction of the disturbance, which, for the harmonic case, is independent of position. If a lattice of vibrating atoms is considered, rather than just a single oscillating atom, a whole spectrum of frequencies is shown to arise in the lattice. Furthermore, in a three-dimensional (3-D) lattice, for every frequency of the spectrum associated with a disturbance in the direction of the wave propagation (a longitudinal wave), there are two vibrational components associated with disturbances perpendicular to the direction of wave propagation (shear waves).

Let us remember, now and throughout this report, that vibrations are the means by which internal (*i.e.*, potential) and kinetic energy are exchanged in a spring. Every type of vibration, no matter how complicated kinematically, has an associated spring constant (or alternately, wave speed) and displacement variable. The derivative of the spring's potential energy with respect to the displacement variable is known as the “force,” and the derivative of the force with respect to this displacement variable is the local spring constant (or stiffness), which governs the vibrational frequency for infinitesimal vibrations of the spring.

An early, important result of lattice-vibration theory was in showing that vibrational energy in a lattice can manifest itself as thermal pressure only if the lattice vibrational frequencies change with lattice deformation—that is to say, if the potential energy well is not parabolic in shape. This condition of nonparabolicity is referred to as anharmonicity. Likewise, nonparabolic terms in a Taylor expansion of the potential energy well about the reference lattice spacing are called anharmonic terms. In practical terms, the empirical metric for anharmonicity usually entails measuring the nonparabolicity of the lattice’s energy well only at the reference lattice spacing (*e.g.*, the method used by Rose *et al.* [3]). Here and throughout this report, the reference condition is one of zero temperature and pressure.

Quantitatively, a lattice’s vibrational energy gets coupled into thermal pressure by way of the Grüneisen function, macroscopically defined as $\Gamma = V(\partial p/\partial E)_V$, where V is the material’s specific volume, and p and E are the pressure and specific energy of the material, respectively. From lattice theory, there is a Grüneisen value associated with each vibrational frequency in the lattice, given by the following expression and taken at constant temperature, T :

$$\Gamma_i = -\frac{V}{\omega_i} \left(\frac{\partial \omega_i}{\partial V} \right)_T , \quad (1)$$

where Γ_i is the Grüneisen value associated with the frequency, ω_i , of a longitudinal or transverse (*i.e.*, shear) vibration. Were the Γ_i values for each frequency truly independent of each other, the macroscopically observed Γ value, being an aggregate of all the Γ_i , would be very difficult to characterize in terms of the individual Γ_i . However, one fortunate simplification to the problem arises from Grüneisen’s assumption, which was originally made based on empirical data and later supported theoretically by the lattice theory of Debye. The assumption asserts that the whole spectrum of lattice vibrational frequencies changes in a characteristically similar fashion with lattice spacing, so that the knowledge of how one characteristic frequency changes with volume defines the behavior of the complete vibrational spectrum. The effect on eqn (1) is to remove the ‘ i ’ subscript, with the resulting equation being characteristic of the behavior of the complete vibrational spectrum. From the early theories of specific heats, this characteristic frequency (a

microscopic quantity) was shown to be directly proportional to a characteristic temperature, Θ (a macroscopic quantity). Thus, it is common to find, in the literature, an interchangeable use of the expressions (ω/ω_0) and (Θ/Θ_0) , where the “0” subscript refers to the reference value. Another simplification is afforded by the approximation, supported by data, that, for solids in the absence of phase change, eqn (1) is independent of temperature, so that the partial derivatives in eqn (1) become ordinary. In this case, Γ , ω , and Θ all become functions of specific volume only. Work in the area of a temperature-dependent Grüneisen function was done by both Blackman [4] and Barron [5], who examined and modeled the variation of Γ with temperature at low values of temperature ($T/\Theta \ll 1$) and found mild variations. Later, Grodzka [6] summarized work, using the compression of porous media, which indicated that some materials (notably aluminum) seem to have a significant decrease in Γ at elevated temperatures. Aluminum aside, the temperature independence of the Grüneisen parameter, while empirical, seems valid over a wide range of conditions and solids.

Even with the simplifications afforded by the temperature-independent, coupled frequency form of eqn (1), the difficulty still arises of how to describe the anharmonic behavior of lattices, given that the prevailing theories describing their fundamental behavior are based on harmonic approximations. Slater [7] and later Dugdale and MacDonald [8] used the harmonic approximation as a basis to develop anharmonic theories of the Grüneisen function.

To better understand the model of Dugdale and MacDonald [8], as well as more recent work, let us construct a framework for analyzing anharmonic vibrations. Given a simple spring-mass system, consider replacing the linear (harmonic) reference spring with a nonlinear (*i.e.*, anharmonic) spring. Vibration theory may be used to compare the frequencies of vibration for these two systems. Though the frequency of vibration for a nonlinear spring changes with amplitude, the situation of low-temperature atomic vibrations may be likened to the situation of a spring experiencing infinitesimal vibrational amplitudes superimposed about a nominal spring extension. In fact, the notion of thermal expansion in a solid is directly analogous to a nonlinear spring, in that, as the temperature is raised, the vibrational amplitude increases, and as the amplitude increases, the nonlinearity of the spring causes the average spring extension (*i.e.*, density) to change, even though the nominal applied force remains constant. The nominal spring extension is analogous, in a lattice, to the atomic spacing relative to the reference

configuration, and the small vibrational oscillations that occur do so about this deformed configuration. Under this condition of infinitesimal vibrations, corresponding to the low-temperature condition of the lattice, the vibrational frequency of a nonlinear spring is obtainable by way of perturbation theory (*i.e.*, by linearizing the problem and considering small perturbations in displacement about the nominal extension). For a given mass, the local spring stiffness determines the vibrational frequency of the spring and is given by the local slope of the force-displacement curve for the spring, which is a function only of the current spring extension. Thus, the relationship that governs how the frequency response is altered by substituting the anharmonic spring for the harmonic reference spring is given as

$$\frac{\omega^2}{\partial F/\partial x} = \frac{\omega_{ref}^2}{\partial F_{ref}/\partial x} = -\frac{1}{M} , \quad (2)$$

where the “*ref*” subscript refers to the reference, harmonic spring.

To further extend the spring analogy to a lattice of atoms, consider the case of a 3-D lattice of spring-connected identical masses. In the general case, the lattice may support physical motion both in the direction of, as well as transverse to, the direction of wave propagation. Furthermore, to be general, we allow the lattice/spring topology to include diagonally connected masses, such that a displacement in one direction may induce force and/or motion in the perpendicular directions. In this general case, the vibrational frequency spectrum of the spring-connected lattice includes components due to both longitudinal and transverse vibrations. Such a frequency spectrum, aggregated of both the longitudinal and transverse spectra, is directly analogous to that found in actual solids. Brillouin [2] has shown that, if a Debye frequency spectrum is assumed for a material, the aggregated characteristic temperature (frequency) is describable as a composite of the longitudinal and transverse frequency spectra as follows:

$$\frac{1}{\Theta_l^3} + \frac{2}{\Theta_t^3} = \frac{3}{\Theta^3} . \quad (3)$$

Others [9, 10] have accomplished a similar result by relating an aggregate of longitudinal and transverse wave-propagation velocities (related to their associated frequency, ω , and wavelength, λ , via $C = \omega\lambda$) directly to the Grüneisen function (related to the frequency spectrum by eqn [1]). For example, Pastine [9] provided this relation as

$$\Gamma = 1/3 [1/3 - (V/C_l) dC_l/dV] + 2/3 [1/3 - (V/C_t) dC_t/dV] , \quad (4)$$

where C_l and C_t refer to the longitudinal and transverse wave speeds, respectively. By relating these component wave speeds to variations in the Poisson ratio, Pastine was able to derive a Grüneisen expression as a function of Poisson's ratio and showed, for the special case of a monatomic face-centered cubic crystal, a result quite close to the theoretically derived result of Barron [5]. However, for the general case, no guidance was offered on appropriate selection of functional forms. Vashchenko and Zubarev [10] adopted a similar approach, but assumed a particular fitting form for the Poisson ratio, in terms of the cold pressure curve and a fitting parameter.

Unlike these other approaches, Plendl [11] considered the measured frequency spectra for real materials, as opposed to using idealized relationships like eqns (3) and (4). Rather than attempting a decomposition of the spectrum into longitudinal and transverse components, he was able to bypass such an approach and show that the characteristic frequency of a material is that frequency at the center of gravity of the frequency spectrum, $f(\omega)$, the so-called "centro-frequency," which is given by

$$\omega_{ctr} = \frac{\int_{\omega_1}^{\omega_2} \omega f(\omega) d\omega}{\int_{\omega_1}^{\omega_2} f(\omega) d\omega} , \quad (5)$$

where the frequency range of integration is selected to comprise the entire range of the acoustical vibration spectrum.

The current analysis follows the lead of Plendl, in that no explicit decomposition of the vibrational spectrum into longitudinal and transverse components will be performed. The mere fact that a characteristic frequency may be aggregated, in some manner, from the longitudinal and transverse frequency spectra (by way of eqn [3], [4], [5], or otherwise) allows us to introduce the concept of a vibrational spring constant, $\partial F_{vib}/\partial x$, which is, by definition, the spring constant that characterizes the aggregated (longitudinal plus transverse) vibrational frequency spectrum. If a lattice had no diagonal coupling and didn't support transverse (shear) waves, the characteristic vibrational stiffness would simply reduce to the stiffness of the component longitudinal spring. The vibrational spring constant will, like the stiffness of a nonlinear spring, be a function of the nominal lattice spacing. By way of this construct of the vibrational spring constant, eqn (2) may be generalized to case of a 3-D coupled lattice:

$$\frac{\omega^2}{\partial F_{vib}/\partial x} = \frac{\omega_{ref}^2}{\partial F_{ref}/\partial x}, \quad (6)$$

where, now, ω is a characteristic frequency of the vibrational spectrum, rather than the specific frequency of the component spring.

Let us analyze a lattice where the specific unit lattice spacings (*i.e.*, length per cube-root unit mass) along the principal lattice directions, x , y , and z , are expressed in terms of the specific volume of the unit cell as $V = \lambda^3 = xyz$, where λ is an averaged unit lattice spacing per cube-root unit mass. For the case of zero-temperature volumetric compression or distention, a specific force may be defined as that force (per 2/3 power unit mass) acting on the face of a unit cell of the lattice, given as $F = p_c \lambda^2 = p_c V^{2/3}$. In this definition, p_c is the cold (0° isotherm) pressure and, thus, the force is positive in compression.

If nothing else were known of the vibrational frequency spectrum, it would be natural to investigate the proportionality of $\partial F_{vib}/\partial x$ and $dF/d\lambda$, since, for a one-dimensional (1-D) harmonic

lattice, these two quantities would, in fact, be identically equal. The assumption that the characteristic vibrational stiffness of a 3-D spring can be made proportional to an associated volumetric stiffness has been pervasive throughout the literature. When Debye theory indicated that the characteristic frequency varied as an aggregate of the elastic wave speeds, Slater [7] assumed a constant Poisson ratio and related the aggregated vibrational stiffness (in terms of wave speeds) directly to volumetric compressibility (although Slater actually concluded something closer to [but not quite] $\omega^2 \sim -dp/d\lambda$ rather than $-dF/d\lambda$). Brillouin [2] derives results utilizing $\omega^2 \sim d^2E_c/d\lambda^2$, the right-hand side being merely $-dF/d\lambda$. It will be shown that Dugdale and MacDonald [8] also utilized this proportionality. More recently, Guinea *et al.* [12] explicitly assumed this proportionality when trying to infer a relationship between the universal cold curve and the Grüneisen function.

The effect of such an assumption of proportionality on eqn (6) is that a $dF/d\lambda$ term may be substituted for each $\partial F/\partial x$. With this substitution, the derivatives with respect to λ are convertible to volume derivatives through the chain rule,

$$dF/d\lambda = dF/dV \cdot dV/d\lambda = (p_c V^{2/3})' \cdot 3V^{2/3} , \quad (7)$$

where the prime symbol ('') denotes ordinary differentiation with respect to specific volume. With this substitution, eqn (6) becomes

$$\frac{\omega^2}{(p_c V^{2/3})'} = \frac{\omega_{ref}^2}{(p_{ref} V^{2/3})'} . \quad (8)$$

If one takes the volume derivative of eqn (8) and divides the result by eqn (8) itself, one obtains

$$2 \frac{d\omega/dV}{\omega} - \frac{(p_c V^{2/3})''}{(p_c V^{2/3})'} = 2 \frac{d\omega_{ref}/dV}{\omega_{ref}} - \frac{(p_{ref} V^{2/3})''}{(p_{ref} V^{2/3})'} . \quad (9)$$

The first term from each side of the equation is related to the Grüneisen function and may be substituted, using the temperature-independent, characteristic-frequency form of eqn (1), to obtain

$$2 \frac{\Gamma}{V} = -\frac{(p_c V^{2/3})''}{(p_c V^{2/3})'} + 2 \frac{\Gamma_{ref}}{V} + \frac{(p_{ref} V^{2/3})''}{(p_{ref} V^{2/3})'} . \quad (10)$$

At this point, the values for the harmonic, reference spring may be substituted. As already mentioned, the value for Γ in a harmonic system is identically zero, since ω is constant, and the last term involving the pressure behavior of the reference system may be acquired using the definition $p_{ref} = -dE_{ref}/dV$, where E_{ref} is the parabolic energy well expressed in terms of V rather than x . The result is the well-known Dugdale-MacDonald relation:

$$\Gamma = -\frac{1}{3} - \frac{V}{2} \frac{(p_c V^{2/3})''}{(p_c V^{2/3})'} . \quad (11)$$

Inserting the harmonic energy potential into this equation results in a Grüneisen value of zero. Such a result illustrates the criticism, by Dugdale and MacDonald [8], of the model of Slater [7]—namely, that inserting the harmonic cold curve into Slater's model does not produce the required value of $\Gamma = 0$.

This report will show, on the basis of Segletes' recently proposed equation of state, that, for a 3-D lattice, the presumed proportionality between the volumetric and vibrational stiffness, which has pervaded the literature and leads to the model of Dugdale and MacDonald, is strictly true only in the harmonic limit of approximation. Force-based, vibrational and volumetric moduli will be compared, for the idealized case of quasi-harmonicity (defined in the next section), with the more general case to be addressed in a subsequent report. Finally, the quasi-harmonic idealization of Segletes' equation of state will be shown to approach the harmonic approximation as the Grüneisen function approaches zero in the limit.

2. Segletes' Equation of State and the Quasi-Harmonic Idealization

Recently, Segletes [13, 14] proposed an equation of state, of Grüneisen form, that properly captures both the lattice-potential and thermal pressure behavior for a variety of crystalline materials, into the megabar range of pressures. The model was inspired by the universal cold curve of Rose *et al.* [3]. However, unlike the model of Rose and other recent equation-of-state models, (*e.g.*, Vinet *et al.* [15, 16]; Baonza, Cáceres, and Núñez [17]; and Baonza *et al.* [18]), the model of Segletes casts the lattice energy potential in terms of the characteristic temperature of the lattice (*i.e.*, the lattice vibrational frequency), rather than lattice spacing (density). The equation of state is given as

$$p\psi - E = E_b \left\{ \left[(\Theta/\Theta_0)^K - 1 \right] + K(K-1)(\Theta/\Theta_0)^K \ln(\Theta/\Theta_0) \right\} . \quad (12)$$

In this equation, p and E are the pressure and specific internal energy respectively, K is a parameter, given by $C_0/(\Gamma_0 \sqrt{E_b})$, where C_0 is the reference bulk sound speed at zero temperature and pressure, E_b is the specific lattice binding energy, and $\psi = V/\Gamma = (\partial E/\partial p)_V$ is a thermodynamic variable introduced by Segletes [19, 20] for ease in manipulating the governing equations. In terms of this variable, ψ , the temperature-independent, coupled-frequency form of eqn (1) is given as

$$\frac{\Theta'}{\Theta} = -\frac{1}{\psi} , \quad (13)$$

where the proportionality between Θ and ω has been utilized. The generalized cold curve associated with eqn (12) is

$$E_c = E_b \{ 1 - (\Theta/\Theta_0)^K [1 - K \ln(\Theta/\Theta_0)] \} \quad (14)$$

and

$$p_c = \frac{E_b K^2}{\Psi} (\Theta/\Theta_0)^K \ln(\Theta/\Theta_0) . \quad (15)$$

When the K parameter takes on a value identically equal to unity and the Grüneisen function varies as $\Gamma \sim V^{1/3}$ (*i.e.*, $\Gamma \sim \lambda$), the equation takes on behavior that will hereafter be called quasi-harmonic. If we denote the variables of the quasi-harmonic equation of state as hatted quantities (^), the quasi-harmonic cold curve becomes

$$\hat{E}_c = \hat{E}_b \{1 - (\hat{\Theta}/\hat{\Theta}_0) [1 - \ln(\hat{\Theta}/\hat{\Theta}_0)]\} \quad (16)$$

with the Grüneisen requirement translating to

$$\hat{\Psi} \sim V^{2/3} . \quad (17)$$

Eqns (16) and (17) are interpreted as quasi-harmonic for a number of reasons. It is immediately obvious that, when K equals unity, many terms drop out from the general equation of state, eqn (12), and the equations become greatly simplified. Furthermore, Segletes and Walters [21, 22] examined the equation of state using a simple power law, V^x , to model the Ψ function. They noted that, over a wide range of anharmonicity, the exponent, x , required to fit well the model of Rose *et al.* [3], varied linearly with Rose's anharmonicity parameter, η . Though it did not match precisely in the limit, an exponential relation of $\Psi \sim V^{2/3}$ was the limiting trend for the case where Rose's anharmonicity, η , approached zero. Segletes and Walters also showed, for the case of $K=1$ and $\hat{\Psi} \sim V^{2/3}$ (the quasi-harmonic case), that the Segletes equation of state satisfies the relation

$$(p_c V^{2/3}) + [2 + 2/3 (\hat{\Psi}/V)] \hat{\Psi} (p_c V^{2/3})' + \hat{\Psi}^2 (p_c V^{2/3})'' = 0 , \quad (18)$$

whereas the Dugdale-MacDonald relation, eqn (11), noted for its harmonic limiting behavior,

satisfies

$$[2 + 2/3 (\psi/V)] \psi (p_c V^{2/3})' + \psi^2 (p_c V^{2/3})'' = 0 . \quad (19)$$

Eqns (18) and (19) differ by only the first term of eqn (18).

In a subsequent report, Segletes will treat the more general form of his equation of state, by showing that the K parameter in eqns (12), (14), and (15) must, for real materials, be a (slowly varying) function of volume, which asymptotes to the quasi-harmonic case in the large-volume limit. In the meantime, the cause of the disparity between the idealized form of Segletes' model and that of Dugdale and MacDonald [8] will be shown to arise from the fact that, for large volumetric strains, the volumetric and vibrational stiffnesses, $dF/d\lambda$ and $\partial F_{vib}/\partial x$, respectively, are not proportional.

3. Force-Based Moduli

The interactions within a lattice are governed by forces acting over distances. On this basis alone, force and distance would seem to be the natural variables governing the interactions within a lattice. More compelling, however, is the fact that Segletes' equation of state shows a very distinct preference for being analyzed in a force-based framework. Eqn (18) is just one example of how, time and again, the term grouping $(p_c V^{2/3})$, which is the force on the face of the lattice unit cell (per 2/3 power unit mass), appears. It is for this reason that subsequent results will be analyzed in a force-based framework, by which it is meant that moduli will be expressed in terms of force gradients, rather than stress gradients. To this end, force-based moduli will be defined for a zero-temperature lattice, at an arbitrary volumetric compression or distention, under the influence of an infinitesimal, superimposed, elastic disturbance.

In a force-based frame, a modulus, with units of stress, may be associated with a given spring constant. From considerations of dimensional analysis, the modulus should be of the form spring constant divided by characteristic length. Alternately, a force-based modulus, associated with the volumetric spring constant, $dF/d\lambda$, for example, may be defined by starting with the stress-based

modulus definition (*i.e.*, bulk modulus), substituting a force term for the stress (pressure) term, and dividing the result by the specific area (*i.e.*, area per 2/3 power mass) over which the force is acting. For a lattice that is only deformed volumetrically, this area is λ^2 , the specific volume to the 2/3 power. Thus,

$$B_F = -\frac{1}{\lambda^2} \frac{dF}{dV/V} = -V^{1/3} \frac{d(p_c V^{2/3})}{dV} = -\frac{1}{3\lambda} \frac{dF}{d\lambda}. \quad (20)$$

Comparison of the stress-based bulk modulus, B , and the force-based one in eqn (20) reveals that, in general, $B_F = B - 2p_c/3$. Under conditions where the pressure and temperature are zero, the force-based volumetric modulus will equal the stress-based bulk modulus in value.

Turning now to the vibrational spring constant, $\partial F_{vib}/\partial x$, an associated force-based modulus, call it J_F , may be defined. As in the case of the vibrational spring constant itself, this modulus implicitly includes the effects of both longitudinal and shear waves. For a cubic lattice, it is given, in terms of λ , by

$$J_F = -\left(\frac{1}{yz} \frac{\partial F_{vib}}{\partial x/x} \right)_{x=y=z=\lambda} = -\frac{1}{\lambda} \frac{\partial F_{vib}}{\partial x}. \quad (21)$$

4. The Relation Between the Volumetric and Vibrational Moduli

We will summarize what is known of the problem at hand by enumerating a list of statements already discussed, so that subsequent reference may conveniently be made to the ideas contained in the following statements:

(1) In a Grüneisen material:

(a) the vibrational spectrum of a lattice is composed of longitudinal and transverse (shear)

vibrational components. This spectrum may be characterized either in terms of characteristic wave speeds or by a characteristic frequency;

- (b) the characteristic frequency of the vibrational spectrum varies with volume in the same manner as the characteristic temperature, $\omega \sim \Theta$; and
 - (c) the characteristic temperature, Θ , is related to the ψ function (and thus Γ) by way of eqn (13).
- (2) The characteristic frequency, ω , of the vibrational spectrum of a lattice may be directly related to an associated spring constant, designated $\partial F_{vib} / \partial x$, of a material, such that the characteristic frequency varies as $\omega^2 \sim \partial F_{vib} / \partial x$. This spring constant may be alternately expressed as a vibrational modulus, designated J_F , and defined in eqn (21).
- (3) The volumetric stiffness, $dF/d\lambda$, is directly derivable from a material's equation of state, and may be alternately expressed in terms of a volumetric modulus, B_F , defined in eqn (20).
- (4) Segletes' equation of state, which fits the behavior of crystalline solids very well, expresses the behavior of the lattice in terms of relative characteristic temperature, Θ/Θ_0 . Since the characteristic temperature (frequency) function is governed by the vibrational stiffness, $\partial F_{vib} / \partial x$, this equation of state may be used to compare directly the volumetric and vibrational stiffnesses.
- (5) Segletes' model, eqn (12), may be idealized to an important special case, termed the quasi-harmonic idealization, which is characterized by:
- (a) a value of the parameter, K , equal to unity; and
 - (b) a ψ function that varies as $V^{2/3}$.

From the cold-pressure curve of Segletes' equation of state, eqn (15), derivatives may be taken, to show that

$$(p_c V^{2/3})' = - \frac{E_b K^2 V^{2/3}}{\psi^2} (\Theta/\Theta_0)^K \left\{ [K + \psi' - 2/3(\psi/V)] \ln(\Theta/\Theta_0) + 1 \right\} . \quad (22)$$

For the quasi-harmonic idealization, defined by statements 5a and 5b, eqn (22) reduces to

$$(p_c V^{2/3})' = - \frac{\hat{E}_b V^{2/3}}{\hat{\psi}^2} (\hat{\Theta}/\hat{\Theta}_0) \left\{ \ln(\hat{\Theta}/\hat{\Theta}_0) + 1 \right\} . \quad (23)$$

If the $\hat{\psi}$ function is quantified as $\hat{\psi} = (V_0^{1/3}/\hat{\Gamma}_0) V^{2/3}$, in accordance with the definition of ψ and statement 5b, then the $dF/d\lambda$ function is given as

$$dF/d\lambda = 3 V^{2/3} (p_c V^{2/3})' = - \frac{3 \hat{E}_b \hat{\Gamma}_0^2}{V_0^{2/3}} (\hat{\Theta}/\hat{\Theta}_0) \left\{ \ln(\hat{\Theta}/\hat{\Theta}_0) + 1 \right\} . \quad (24)$$

We see here why the quasi-harmonic case is an important one—namely, because the interatomic force and its spacial derivatives vary only with the characteristic frequency and not explicitly as a function of lattice spacing (λ or V). The relative ratios of the zero-temperature vibrational and volumetric stiffnesses may be compared as a function of characteristic temperature ratio and are displayed in Figure 1. The upper curve, for vibrations, is parabolic since (according to statements 1b and 2) it is the spring constant which governs the characteristic frequency (and thus characteristic temperature). The lower curve, derived from Segletes' model for the quasi-harmonic case, relates the relative volumetric stiffness to the characteristic temperature. Were these two curves to overlay, the model of Dugdale and MacDonald [8] would prevail. As it is, the vibrational and volumetric stiffnesses for a quasi-harmonic, 3-D lattice do not remain proportional, though they do so approximately near the reference density.

Eqn (24) expresses the volumetric stiffness in terms of the quasi-harmonic, characteristic temperature of the lattice. A converse relationship may be obtained by starting with eqn (18), and making the substitution in the bracketed term that, for the quasi-harmonic case,

$\Psi' = 2/3 (\hat{\Psi}/V)$. Employing the fact that $F = p_c V^{2/3}$, the resulting equation may be rearranged to give

$$-\frac{1}{\hat{\Psi}} = \frac{(\hat{\Psi}F'' + (1 + \hat{\Psi}')F')}{(\hat{\Psi}F' + F)} . \quad (25)$$

The left side of the equation is, by way of eqn (13), $\hat{\Theta}'/\hat{\Theta}$. Similarly, the numerator of the right side of the equation is also the volume derivative of the denominator. Thus, we see that

$$\hat{\Theta}' \sim \hat{\Psi}F' + F = \frac{\lambda_0}{3 \hat{\Gamma}_0} \frac{dF}{d\lambda} + F , \quad (26)$$

which expresses the characteristic frequency in terms of the lattice cell force and its spacial derivative.

To put the comparison in yet another perspective, in terms of the moduli, we compute, from eqns (20) and (24), that $\hat{B}_F/\hat{B}_{0F} = (\lambda_0/\lambda)(\hat{\Theta}/\hat{\Theta}_0)[\ln(\hat{\Theta}/\hat{\Theta}_0) + 1]$. Likewise, from eqn (21) and statements 1b and 2, we know that $\hat{J}_F/\hat{J}_{0F} = (\lambda_0/\lambda)(\hat{\Theta}/\hat{\Theta}_0)^2$. We will assume now the initial condition, that $\hat{J}_{0F} = \hat{B}_{0F}$. This assumption corresponds, for a 3-D lattice, to the situation where $(dF/d\lambda)_{V_0}$ equals $3(\partial F_{vib}/\partial x)_{V_0}$. If this assumption should subsequently prove wrong, the sole effect will be that eqns (27) and (30), to follow, will be off by a constant multiplier. The force-based volumetric and vibrational moduli, for the quasi-harmonic case, may thus be directly related as

$$\hat{B}_F/\hat{J}_F = \frac{[\ln(\hat{\Theta}/\hat{\Theta}_0) + 1]}{(\hat{\Theta}/\hat{\Theta}_0)} . \quad (27)$$

A graph of this function is shown in Figure 2, as a function of the quasi-harmonic, relative characteristic temperature, $\hat{\Theta}/\hat{\Theta}_0$. This figure indicates the functional relationship between the force-based volumetric and vibrational moduli for the quasi-harmonic case.

Alternately, this relationship may be expressed as a function of specific volume ratio, by converting characteristic temperature to specific volume. By starting with the quasi-harmonic ψ function, given by

$$\hat{\psi} = (V_0^{1/3}/\hat{\Gamma}_0) V^{2/3} , \quad (28)$$

one may integrate according to eqn (13) to ascertain the logarithm of the quasi-harmonic frequency function:

$$\ln(\hat{\Theta}/\hat{\Theta}_0) = 3 \hat{\Gamma}_0 [1 - (V/V_0)^{1/3}] . \quad (29)$$

Interestingly, the quasi-harmonic eqn (29) is proportional to the negative of the a^* parameter employed by Rose *et al.* [3], as the nondimensional lattice parameter in their universal cold curve. The model of Rose *et al.*, which was the inspiration for Segletes' equation of state [13, 14], expresses cold energy in terms of compression and is seen from eqn (29) to relate closely to the quasi-harmonic case idealized from Segletes' model. However, unlike Segletes' equation of state, Rose's model does not include thermal pressure effects required for a complete equation of state and has no provisions for Segletes' general case, which is not quasi-harmonic.

Exponentiation of eqn (29) provides the characteristic temperature ratio. The quasi-harmonic characteristic temperature ratio tells exactly why the real world is not quasi-harmonic—because, in the quasi-harmonic case, there is a maximum limiting frequency ratio at vanishingly small volumes, given by $(\hat{\Theta}_{\max}/\hat{\Theta}_0) = \exp(3\hat{\Gamma}_0)$. Such a frequency limit would translate into a cold-compression energy limit, as well. According to various high-compression theories that include electronic effects, finite cold-compression energies under infinite compression do not occur in actual materials. Such limiting compressive behavior, though absent in actual materials,

characterizes both the model of Rose *et al.* [3], as well as the quasi-harmonic idealization. A subsequent report will address how actual materials may be described by Segletes' theory, by departing from the tenets of the quasi-harmonic idealization. In the report to appear, the author intends to show that the data support the notion that, as lattice spacing increases, the behavior of all lattices approaches the quasi-harmonic idealization, and that a departure from this ideal occurs as the lattice spacing becomes small enough to permit interatomic repulsive interactions.

Substitution may be made into eqn (27), in order to express the volumetric to vibrational modulus ratio, in terms of specific volume, as

$$\hat{B}_F/\hat{J}_F = \frac{\{1 + 3\hat{\Gamma}_0[1 - (V/V_0)^{1/3}]\}}{\exp\{3\hat{\Gamma}_0[1 - (V/V_0)^{1/3}]\}} . \quad (30)$$

This relationship is depicted in Figure 3 with the reference, quasi-harmonic Grüneisen parameter value, $\hat{\Gamma}_0$, as a parameter. The figure shows that, only as $\hat{\Gamma}_0$ is made to approach zero, does the quasi-harmonic, zero-temperature, volumetric to vibrational modulus ratio approach a constant value (of unity). The quasi-harmonic lattice force, $F = (p_c V^{2/3})$, may also be expressed in terms of lattice spacing, rather than frequency, through the use of eqns (15) and (29) and the definition that $\lambda = V^{1/3}$.

$$F = \hat{E}_b(\hat{\Gamma}_0/\lambda_0) \exp[3(\hat{\Gamma}_0/\lambda_0)(\lambda_0 - \lambda)] [3(\hat{\Gamma}_0/\lambda_0)(\lambda_0 - \lambda)] . \quad (31)$$

It is also revealing to study the quasi-harmonic, cold-energy curve, not as a function of frequency, as given in eqn (16), but likewise in terms of relative lattice spacing, using eqn (29) and the relation between λ and V . Figure 4 plots this relation with the reference quasi-harmonic Grüneisen parameter, $\hat{\Gamma}_0$, as a parameter. The energy has been normalized by its limiting ($V = 0$) cold-compression energy, which is finite for the quasi-harmonic case, but will not be so for real materials. The figure clearly shows that, as the reference Grüneisen parameter approaches zero, the quasi-harmonic idealization of Segletes' equation approaches the harmonic case, consistent

with Dugdale and MacDonald [8] theory, as already shown for $\Gamma = 0$. Kittel [23] indicates that, according to harmonic theory, there is no thermal expansion, and the elastic constants are independent of pressure (and temperature). A zero Grüneisen function follows from a zero thermal-expansion coefficient. Thus, the constant ratio of the elastic moduli in Figure 3, for the limiting case of $\hat{\Gamma}_0 = 0$, is further evidence of compatibility with harmonic theory. Furthermore, $\partial F_{vib}/\partial x$ and $dF/d\lambda$ are proportional for only this limiting case and this proportionality is exactly what would occur for a 3-D lattice of atomic masses connected by simple linear springs. In short, the quasi-harmonic idealization approaches the harmonic limit as $\hat{\Gamma}$ approaches zero.

The harmonic condition has been traditionally expressed by stipulating the potential energy well to be parabolic,

$$\frac{d^3 E_{pot}}{d\lambda^3} = 0 \quad , \quad (32)$$

thus resulting in a constant characteristic frequency and an identically zero Grüneisen function. We see now that the harmonic approximation is merely the limiting case of the quasi-harmonic idealization of Segletes' equation of state, when the value of the Grüneisen function is made to approach zero in the limit. The quasi-harmonic potential, given by eqn (16), satisfies the following relation:

$$\frac{d^2}{d\lambda^2} \left(\frac{\hat{E}_{pot}}{\Theta} \right) = 0 \quad , \quad (33)$$

where E_{pot} , the potential energy well of the lattice, is the lattice cold energy relative to the infinite lattice separation condition, or $E_{pot} = E_c - E_b$.

5. Conclusions

The historical use of the harmonic approximation in the study of lattice dynamics has been briefly reviewed to include the development of the Dugdale-MacDonald model of anharmonic lattice behavior. It is shown how, in the case of the model of Dugdale and MacDonald [8], results rely on a certain assumption about the governing elasticity—an assumption that follows from 1-D theory wherein the vibrational and volumetric stiffnesses are proportional. This assumption has been widely adopted by prior treatments of the subject, but has been shown to be inadequate to describe the behavior of a 3-D lattice at large volumetric strain, perhaps as a result of lateral (Poisson ratio) coupling, transverse (shear) waves and/or the presence of non-nearest neighbor interatomic interactions.

The relationship between vibrational and volumetric moduli has been studied using the quasi-harmonic idealization of Segletes' equation of state. The quasi-harmonic idealization is one in which the form of Segletes' equation of state is greatly simplified, while the Grüneisen function takes on a specified, idealized, functional behavior. In the quasi-harmonic idealization, the interatomic force and its spacial derivatives vary only with the characteristic frequency of the lattice and not explicitly with the lattice spacing.

Results indicate that the relationship between the vibrational and volumetric moduli (and their associated natural frequencies) are of different form. In the vibrational case, the stiffness, according to vibration theory, goes as ω^2 , whereas for volumetric distortions of a 3-D lattice, it may be inferred from the idealized form of Segletes' equation of state that the volumetric stiffness goes as $\omega[1 + \ln(\omega/\omega_0)]$. It is this disparity that causes the primary difference between the model of Segletes and previous work by Dugdale and MacDonald [8].

The idealized Grüneisen relationship that governs quasi-harmonic behavior is such that a quasi-harmonic lattice reaches a limiting cold-compression energy (and associated vibrational frequency) in the limit of vanishingly small volume. Such idealized behavior, though not indicative of real materials, is compatible with the theory of harmonic lattice vibrations. This

report explicitly shows that the quasi-harmonic idealization, for the limiting case where the Grüneisen function approaches zero, actually approaches the harmonic approximation.

In a subsequent report, the author intends to address how real material behavior may be described in the framework of Segletes' equation of state, by departing from the quasi-harmonic idealization, and how, as lattice spacing increases, the quasi-harmonic idealization is approached for real lattices. Such a result is wholly compatible with the conclusions of Pendl [11], who asserts that anharmonicity is "mainly caused by the forces of repulsion..., but is close to zero when ions deviate from one another," (*i.e.*, when $\lambda > \lambda_0$).

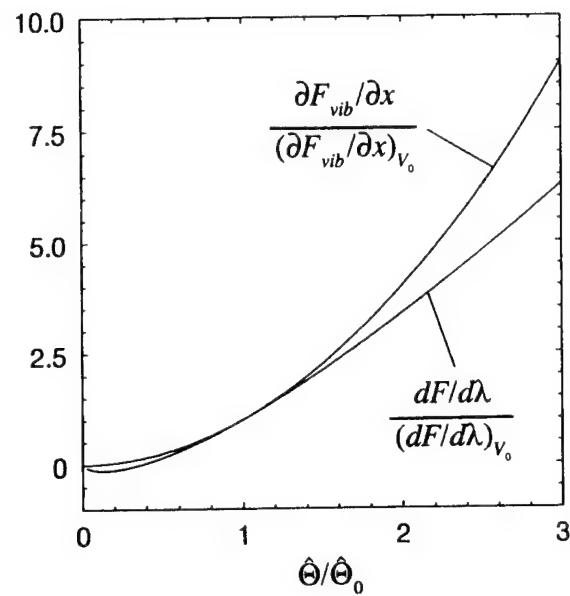


Figure 1. Relative values of the vibrational ($\partial F_{vib}/\partial x$) and volumetric ($dF/d\lambda$) stiffnesses, as a function of the relative characteristic temperature (or frequency), for a material obeying the quasi-harmonic idealization.

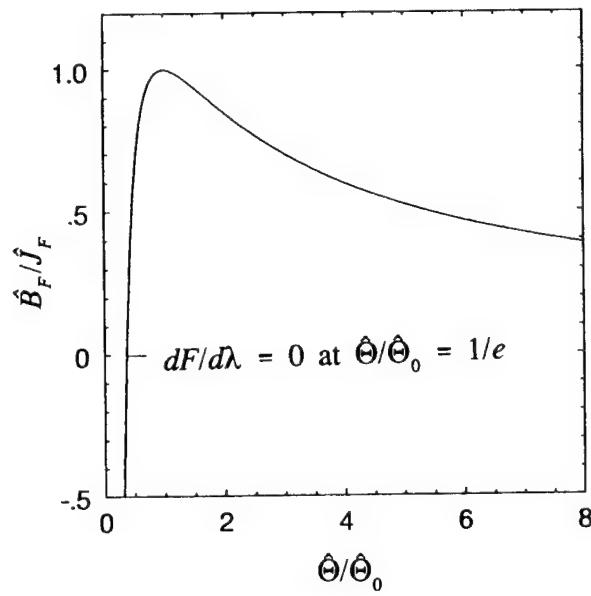


Figure 2. Ratio of volumetric to vibrational (force-based) moduli, as a function of the relative characteristic temperature (or frequency), for a material obeying the quasi-harmonic idealization.

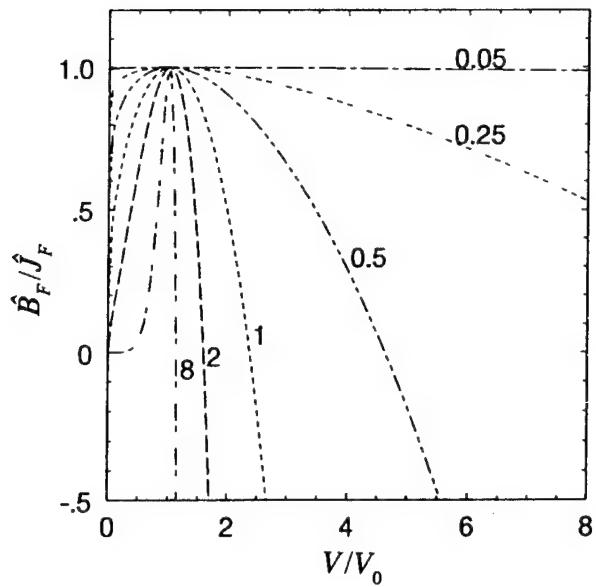


Figure 3. Ratio of volumetric to vibrational (force-based) moduli, as a function of relative volume, for a material obeying the quasi-harmonic idealization. Six curves are shown, corresponding to different values of the reference Grüneisen parameter, Γ_0 .

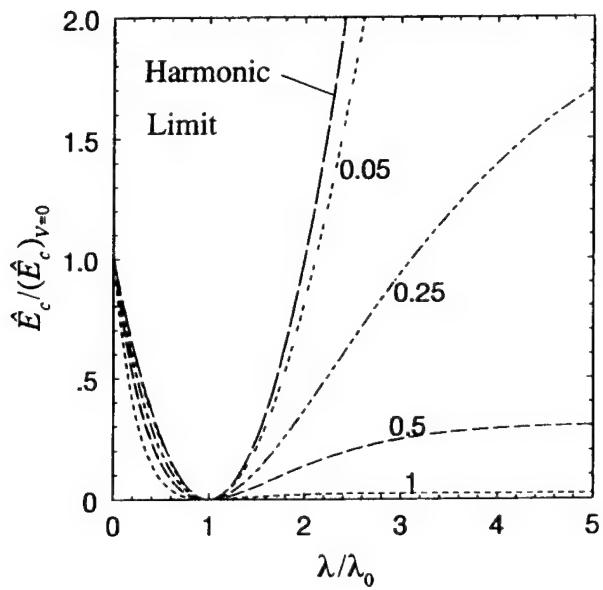


Figure 4. Relative cold compression energy versus relative lattice spacing, with reference Grüneisen value, Γ_0 , as a parameter, for quasi-harmonic material. As Γ_0 approaches zero, harmonicity is approached.

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13. ABSTRACT (Maximum 200 words)

The implications of Segletes' recent equation of state are examined, when idealized to the condition defined as quasi-harmonicity. Results indicate that at large volumetric strains, a proportionality no longer holds, in general, between the volumetric and vibrational stiffnesses. The governing relation between these two stiffnesses is presented and is a function of the characteristic frequency of the lattice, alternately expressed in terms of the lattice spacing. It is further shown that the quasi-harmonic idealization of Segletes' equation will approach the harmonic approximation in the limit.

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5. Has the information in this report led to any quantitative savings as far as man-hours or dollars saved, operating costs avoided, or efficiencies achieved, etc? If so, please elaborate.

6. General Comments. What do you think should be changed to improve future reports? (Indicate changes to organization, technical content, format, etc.)

Organization

CURRENT
ADDRESS

Name

E-mail Name

Street or P.O. Box No.

City, State, Zip Code

7. If indicating a Change of Address or Address Correction, please provide the Current or Correct address above and the Old or Incorrect address below.

Organization

OLD
ADDRESS

Name

Street or P.O. Box No.

City, State, Zip Code

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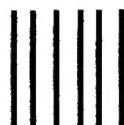
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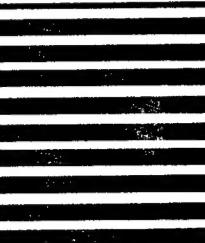
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